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DEPARTMENT OF MATHEMATICAL SCIENCES
COLLEGE OF SCIENCES
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA 23529

THEORETICAL STUDIES OF SOLAR LASERS AND CONVERTERS

By

John H. Heinbockel, Principal Investigator

Progress Report
For the period May 15 to December 31, 1988

Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia 23665-5225

Under
Research Grant NAG-1-757
Dr. R.C. Costen, Technical Monitor
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Theoretical Studies of Solar Lasers and Converters

A second computer program has been developed for the simulation of an $n-C_3F_7I$ iodine laser. This computer program is given in the Appendix A and typical output from the computer program is illustrated in the Appendix B.

Chemical Kinetics

The computer program simulates the chemical kinetics occurring during the operation of an $n-C_3F_7I$ iodine laser. Letting R denote the radical $n-C_3F_7$, these reactions are summarised as follows:

Photodissociation of RI and I_2:

$$RI + h\nu_1 \xrightarrow[\xi_1]{0.27\mu m} R + I^*$$

$$I_2 + h\nu_2 \xrightarrow[\xi_2]{0.5\mu m} I + I^*$$

Laser action (stimulated emission)

$$I^* + h\nu_3 \xrightarrow{1.32\mu m} I + 2h\nu_3$$

Quenching of I^* (reaction rates have units $[cm^3/sec]$)

$$I^* + RI \xrightarrow{Q_1} I + RI$$

$$I^* + I_2 \xrightarrow{Q_2} I + I_2$$

$$I^* + R \xrightarrow{Q_3} I + R$$

$$I^* + R_2 \xrightarrow{Q_4} I + R_2$$

$$I^* + I \xrightarrow{Q_5} I + I$$

RI generation and two body recombinations (reaction rates have units $[cm^3/sec]$)

$$R + I^* \xrightarrow{k_1} RI$$

$$R + I \xrightarrow{k_2} RI$$

$$R + R \xrightarrow{k_3} R_2$$

$$R + RI \xrightarrow{k_4} R_2 + I$$

$$R + I_2 \xrightarrow{k_5} RI + I$$

$$R + RI \xrightarrow{k_6} R_2 + I^*$$

$$RI + I^* \xrightarrow{k_7} I_2 + R$$

$$I + RI \xrightarrow{k_8} I_2 + R$$

I_2 formation (reaction rates have units $[cm^3/sec]$)

$$I^* + I + RI \xrightarrow{c_1} I_2 + RI$$
$$I + I + RI \xrightarrow{c_2} I_2 + RI$$
$$I^* + I + I_2 \xrightarrow{c_3} I_2 + I_2$$
$$I + I + I_2 \xrightarrow{c_4} I_2 + I_2$$
$$I + I + R_2 \xrightarrow{c_5} I_2 + R_2$$
$$I + I^* + R_2 \xrightarrow{c_6} I_2 + R_2$$

Wall reactions (reaction rates have units $[cm^3/sec]$)

$$I + I + wall \xrightarrow{v_1} I_2 + wall$$
$$R_2 + I + wall \xrightarrow{v_2} R + RI + wall$$

Reaction rate coefficients

The reaction rate coefficients are assumed to satisfy the following inequalities:

$$.476(10^{-16}) \leq Q_1 \leq 8.4(10^{-16})$$
$$.730(10^{-11}) \leq Q_2 \leq 4.94(10^{-11})$$
$$1.23(10^{-18}) \leq Q_3 \leq 11.1(10^{-18})$$
$$1.57(10^{-16}) \leq Q_4 \leq 14.1(10^{-16})$$
$$.530(10^{-14}) \leq Q_5 \leq 4.8(10^{-14})$$

$$0.9(10^{-13}) \leq k_1 \leq 34.7(10^{-13})$$
$$.657(10^{-11}) \leq k_2 \leq 8.05(10^{-11})$$
$$.65(10^{-12}) \leq k_3 \leq 10.4(10^{-12})$$
$$1.0(10^{-16}) \leq k_4 \leq 9.0(10^{-16})$$
$$0.33(10^{-11}) \leq k_5 \leq 3.0(10^{-11})$$
$$1.0(10^{-17}) \leq k_6 \leq 10.24(10^{-17})$$
$$1.5(10^{-19}) \leq k_7 \leq 4.5(10^{-19})$$
$$0.533(10^{-23}) \leq k_8 \leq 4.8(10^{-23})$$

$$1.0(10^{-33}) \leq c_1 \leq 10.2(10^{-33})$$
$$1.6(10^{-32}) \leq c_2 \leq 45.0(10^{-32})$$
$$4.44(10^{-32}) \leq c_3 \leq 14.4(10^{-32})$$
$$2.92(10^{-30}) \leq c_4 \leq 4.94(10^{-30})$$
$$3.6(10^{-31}) \leq c_5 \leq 6.0(10^{-31})$$
$$1.35(10^{-32}) \leq c_6 \leq 2.25(10^{-32})$$

$$0.33(10^{-12}) \leq v_1 \leq 3.0(10^{-12})$$
$$0.33(10^{-11}) \leq v_2 \leq 3.0(10^{-11})$$

Other coefficients

In the computer program we let: Q_y denote the quantum yield; ξ_1, ξ_2 denote the photodissociation rates which are dependent upon the solar simulator concentration c_0; σ denotes the stimulated emission cross section and ρ denotes the photon density in the optical cavity. We use the approximations

$$\xi_1 = 3.04(10^{-3})c_0, \qquad \xi_2 = 3.38(10^{-2})c_0$$

The pumping is assumed to occur over an interval $0 \le z \le z_L$ where L is the length of the tube. Various assumptions can be incorporated concerning the pumping intensity. Currently, the program assumes that the maximun pumping intensity occurs at $z_{0L} = \frac{1}{2}z_L$.

Differential equations for chemical kinetics

Using the notation $[A]$ to denote the concentration of species A in units of cm^{-3}, the differential equations defining the chemical kinetics for the iodine lase can be expressed by the following set of coupled nonlinear differential equations involving the concentrations $[RI]$, $[R]$, $[R_2]$, $[I_2]$, $[I^*]$, $[I]$.

$$\begin{aligned}
\frac{d[RI]}{dt} &= k_1[R][I^*] + k_2[R][I] + k_5[R][I_2] - k_7[I^*][RI] - k_4[R][RI] \\
&\quad - k_6[R][RI] - \xi_1[RI] + v_2[R_2][I] - k_8[I][RI] \\
\frac{d[R]}{dt} &= \xi_1[RI] - k_1[R][I^*] - k_2[R][I] - 2k_3[R]^2 - k_4[RI][R] \\
&\quad - k_6[RI][R] - k_5[R][I_2] + v_2[R_2][I] + k_7[RI][I^*] + k_8[I][RI] \\
\frac{d[R_2]}{dt} &= K_3[R]^2 + k_6[RI][R] + k_4[RI][R] - v_2[R_2][I] \\
\frac{d[I_2]}{dt} &= c_1[RI][I^*][I] + c_2[RI][I]^2 + c_3[I_2][I^*][I] + c_4[I_2][I]^2 \\
&\quad - \xi_2[I_2] + k_7[RI][I^*] - k_5[R][I_2] + v_1[I]^2 \\
&\quad c_5[I]^2[R_2] + k_8[RI][I] + c_6[I][I^*][R_2] \\
\frac{d[I^*]}{dt} &= Q_y\xi_1[RI] + \xi_2[I_2] - k_1[R][I^*] - Q_2[I_2][I^*] \\
&\quad - c\sigma\rho([I^*] - \frac{1}{2}[I]) + k_6[R][RI] - Q_3[R][I^*] - Q_4[R_2][I^*] \\
&\quad - Q_5[I^*][I] - k_7[RI][I^*] - C_6[R_2][I^*][I] - C_1[RI][I^*][I] \\
&\quad - C_3[I_2][I^*][I] - Q_1[RI][I^*] \\
\frac{d[I]}{dt} &= \xi_2[I_2] + Q_1[RI][I^*] + Q_2[I_2][I^*] - 2c_5[I]^2[R_2] - k_8[I][RI] \\
&\quad + c\sigma\rho([I^*] - \frac{1}{2}[I]) - c_1[RI][I^*][I] - 2c_2[RI][I]^2 - c_3[I_2][I^*][I] \\
&\quad + 2c_4[I_2][I]^2 - k_2[R][I] + k_4[RI][R] + Q_3[I^*][R] + Q_4[I^*][R_2] \\
&\quad + Q_5[I^*][I] + k_5[R][I_2] - v_2[R_2][I] - 2v_1[I]^2 - c_6[R_2][I^*][I]
\end{aligned}$$

In the above differential equations we use the material derivative

$$\frac{d[A]}{dt} = \frac{\partial[A]}{\partial t} + \frac{\partial[A]}{\partial z}\frac{dz}{dt} = \frac{\partial[A]}{\partial t} + \frac{\partial[A]}{\partial z}\omega$$

where $\frac{dz}{dt} = \omega$ is the flow rate in the axial direction

The above system of nonlinear differential equations conserves the masses of the species involved in the reactions and for steady state operation at any point z we have the immediate integrals

$$[RI] + [R] + 2[R_2] = constant$$
$$[RI] + 2[I_2] + [I^*] + [I] = constant$$

Photon density

For the light flux density of lasing photon ρ we let $\rho = \rho_+ + \rho_-$ where $\rho_+ = \rho_+(z,t)$ denotes the photon density propagating in the positive z direction and $\rho_- = \rho_-(z,t)$ denotes the photon density propagating in the negative z direction. The differential equations for these photon densities are given by

$$\frac{1}{c}\frac{\partial \rho_+}{\partial t} + \frac{\partial \rho_+}{\partial z} = \sigma[I^*]\,\rho_+ ([I^*] - \frac{1}{2}[I])$$
$$\frac{1}{c}\frac{\partial \rho_-}{\partial t} - \frac{\partial \rho_-}{\partial z} = \sigma\rho_- ([I^*] - \frac{1}{2}[I])$$

where c is the speed of light in the optical medium. In the above equations $\sigma[I^*]\rho_+$ is the amplification factor resulting from population of the upper lasing level of the active medium and $-\frac{1}{2}\sigma[I]\rho_+$ is the decrease in photon density due to population of the lower lasing level.

Compressible flow

The effects of fluid density variation as a function of distance z along the tube is considered. Also the pressure and temperature of the flow medium are calculated as a function of distance z and incorporated into the computer model by including the following equations:

(i) An equation of state:

For P the pressure in the gas, T the absolute temperature, and η the gas density, we assume an equation of state for a perfect gas

$$P = \eta RT$$

where R is the universal gas constant.

(ii) Continuity equation (conservation of mass):

The continuity equation is expressed

$$\frac{\partial \eta}{\partial t} + div\,(\eta \vec{V}) = 0$$

where η is the gas density and $\vec{V}$ is the gas velocity. For steady state conditions and $\vec{V} = \omega \hat{k}$ the flow in the axial direction, the continuity equation reduces to

$$\frac{\partial}{\partial z}(\eta\omega) = 0$$

which implies that

$$\eta\omega = constant.$$

(iii) Momentum equation

The momentum equation for a control volume having a mass $\eta d\tau$ where $d\tau$ is an element of volume, is given by

$$\vec{M} = \iiint \vec{V}\,\eta\, d\tau.$$

Using Newton's second law we have

$$\vec{F} = \frac{D\vec{M}}{Dt} = \frac{D}{Dt}\iiint \vec{V}\,\eta\, d\tau$$

where $\frac{D}{Dt}$ is the material derivative. We have that

$$\frac{D\vec{M}}{Dt} = \iint \vec{V}(\eta\vec{V}\cdot d\vec{\sigma}) + \frac{\partial}{\partial t}\iiint \vec{V}\,\eta\, d\tau$$

where the surface integral term above represents the efflux of momentum through the control volume and the volume integral term represents the change in momentum inside the control volume. Changing the surface integral to a volume integral by using the Gauss divergence theorem

$$\iint \vec{V}(\eta\vec{V}\cdot d\vec{\sigma}) = \iiint \left[\nabla\cdot\eta\vec{V}\vec{V}\right] d\tau$$

and letting $\vec{F} = \iiint \vec{f}\, d\tau$ where $\vec{f}$ is the average force per unit volume, we obtain

$$\vec{F} = \iiint \vec{f}\, d\tau = \iiint \left[\frac{\partial}{\partial t}(\eta\omega)\hat{k} + \frac{\partial}{\partial z}(\eta\omega^2)\hat{k}\right] d\tau$$

where $\vec{V}\vec{V} = \omega^2\hat{k}\hat{k}$ is a dyadic and $\vec{f} = -\nabla P$ is the average force per unit volume which is due to the fluid pressure P. This equation implies that

$$-\frac{\partial P}{\partial z} = \frac{\partial}{\partial t}(\eta\omega) + \frac{\partial}{\partial z}(\eta\omega^2).$$

Using the result $\eta\omega = c_1 =$ a constant, the steady state form of the above gives us

$$-\frac{\partial P}{\partial z} = c_1\frac{\partial \omega}{\partial z}$$

and an integration gives

$$P + c_1\omega = c_2$$

where c_2 is a constant of integration.

Energy equation

In terms of the specific enthalpy h per unit mass, the energy equation for the gas flow can be expressed

$$\eta\frac{Dh}{Dt} = \frac{DP}{Dt} + \kappa\nabla^2 T + q$$

where P is the pressure, T is the absolute temperature, κ is the thermal conductivity, and $q = q(z)$ is the raditation heat flux. In one dimension, the energy equation can be expressed

$$\eta\frac{\partial h}{\partial t} + \eta\omega\frac{\partial h}{\partial z} = \frac{\partial P}{\partial t} + \omega\frac{\partial P}{\partial z} + \kappa\frac{d^2T}{dz^2} + q.$$

For C_p the specific heat at constant temperature and C_v the specific heat at constant volume, we can write $h = C_pT$ and $C_p - C_v = R$. This gives us the steady state equation

$$\eta\omega[C_v(T) + R]\frac{dT}{dz} = \omega\frac{dP}{dz} + \kappa\frac{d^2T}{dz^2} + q$$

where we have neglected the effects of viscosity. If we also neglect the effects of the thermal conductivity the above equation reduces to

$$c_1[C_v(T) + R]dT + \omega c_1 d\omega + q dz = 0$$

Using the empirical model

$$C_v(T) = \alpha_v \exp(\beta_v(T - 300)), \qquad 298.15 \le T \le 500$$

where $\alpha_v = 147.23$ and $\beta_v = 0.0012$ are constants, the above equation can be integrated to obtain

$$c_1\frac{\alpha_v}{\beta_v}\exp(\beta_v(T - 300)) + c_1R(T - 300) + \frac{1}{2}c_1\omega^2 - Q = c_4$$

where

$$Q = \int q(z)\, dz$$

and c_4 is a constant of integration.

Computer program

The above equations can be found in the computer program listed in the Appendix A. This program can be described as follows:

Main program

This assigns values to all constants and parameters and then guesses at an initial photon density. The equations are then integrated from 0 to L and the boundary conditions (discussed in an earlier report) are checked to see if they are satisfied. If they are not satisfied then an iterative scheme is employed to find the initial photon density which satisfies the boundary conditions. When the correct initial photon density is used the results of the computations are printed out.

Subroutine GRAPHS

Produces graphical output for each of the species concentration as a function of distance z in the axial direction.

Subroutine PFLOW

This subroutine calculates certain parameters needed in subroutine FLOW. These parameters are stored in common BLK10.

Subroutine FLOW

This subroutine calculates the temperature T, pressure P, flow rate W, density η, Pressure in torr, as a function of axial distance z.

Subroutine ARREN

This subroutine calculates how some of the rate coefficients change with temperature where we have assumed various arrenhius expressions for the different rate coefficients. Other rate coefficients are held constant.

Subroutine CHSI1

This subroutine calculates ξ_1 as a function of z.

Subroutine CHSI2

This subroutine calculates ξ_2 as a function of z.

Subroutine COEFFS

This subroutine calculates the various constants and rate coefficients needed for execution of the program.

Subroutine VELOC

This subroutine calculates the velocity ω as a function of tube radius. Various assumed flow patterns can be assumed. Current version assumes a parabolic flow profile with the velocity of the gas going to zero at the tube walls.

Subroutine FUN

This subroutine calculates the functions occuring on the right hand side of the differential equations to be solved.

Subroutine SIGMA

This subroutine calculates the abeorption cross section σ.

Subroutine INTEG

This subroutine integrates the differential equations from 0 to z using a 7th order Runge-Kut'a-Fehlberg variable step size integration routine.

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APPENDIX A

```
      PROGRAM CFLM1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)
C     MAIN PROGRAM
C     COMPRESSIBLE FLOW LASER MODEL WHICH INCLUDES
C          EQUATION OF STATE
C          CONTINUITY EQUATION
C          MOMENTUM EQUATION
C          ENERGY EQUATION
C
C         USED IN PREDICTION MODE---GIVEN CONDITIONS AT Z=0.
C
C
C     THIS VERSION CONTAINS AN AUTOMATICALLY CHOSEN VARIABLE STEP
C     SIZE.  IT ALSO CONTAINS WALL EFFECT REACTIONS.(NOT USED THOUGH)
C
C      EFFECTS OF TEMPERATURE, FLOWRATE,DENSITY AND PRESSURE VARIATIONS
C      ARE CONSIDERED IN SUBROUTINES APREN, PFLOW AND FLOW
      COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
      COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
      COMMON/BLK3/B,B2,B3,C,AUO,BOO,EPSNU,OMEGA,C6
      COMMON/BLK4/CHSI1O,CHS12O,ABARO,Z1BAR,LC
      COMMON/BLK7/ABC,COO,CO,OMEG1,P,R1,R2,TM,XNRHO
       COMMON/BLK8/ZUL,ZE,NG,TO,RAD,A
       COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AAO,BBO
      COMMON/BLK22/AD,V1,V2,GG
      COMMON/BLK23/WO,ETAO,PTO,FRAC
      REAL K1,K2,K3,K4,K5,K6,K7,K8
       REAL LC,L
       WRITE(6,123)
  123  FORMAT(1X,20H START OF PROGRAM          )
C      DEFAULT VALUES
      IEND=0
      ICOUNT=0
      NG=0
      FRAC=.018
       AR=2.
       TLE=39.0
       PTO=25.0
       WO=15.8
       ETAO=.38
       T=TLE+273.
      ZOL=7.50
       AAO=147.23
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```
                BBO=.0012
              C  AAO,BBO USED IN LEAST SQ FIT OF SP.HEAT CONSTANT VOLUME
45            P=40.
             LC=6.0
              XNRHO=1.0
             RAD=0.C
             COO=.5E25
50            R1=.9975
              R2=.975
              ZE=5.0
             A=1.0
              TM= 1-R2
55            OMEG1=5000.
              CON=2.0E4
             NAMELIST/PARAM/PTO,OMEG1,CON,COO,R1,R2,TM,XNPHO,LC,ZOL,A,ZE,
            1  AR, IEND ,FRAC ,T,PTO,RAD
              C  ASSUME PRESSURE PTO (TORR) AND TEMPERATURE T (DEG K)
60            C  ARE GIVEN FOR LEFT END.  CALCULATE ETAO TO SATISFY GAS LAW
              55  CONTINUE
             IF(IEND .EQ. 1) GO TO 600
             IF(NG.EQ.8) GO TO 600
              ICOUNT=ICOUNT+1
65            READ(5,PARAM)
              IF(EOF(5))600,601
             600  WRITE(6,603)
             603  FORMAT(1X,28HEND OF FILE ENCOUNTERED-STOP)
              CALL PSEUDO
70            DO 10 JJJ=1,5
              CALL GRAPHS(JJJ)
             10  CONTINUE
              STOP 1313
              C  P=PRESSURE, TORR
75            C  AR=LASER BEAM DIAMETER CM
              C  A=RADIUS OF TUBE (CM)
              C  RAD=RADIUS OF TUBE WHERE CALCULATIONS ARE DONE.
              C  T=TEMPERATURE DEG K
              C  TO=TEMPERATURE LEFT END DEG K
80            C  PTO= PRESSURE TORR LEFT END
              C  WO=FLOW RATE LEFT END M/SEC
              C  ETAO=DENSITY OF GAS KG/M**3
              C  OMEG1=FLOW RATE, CM/SEC , MAXIMUM FLOW RATE AT RAD=0
              C  CON=PEAK CONCENTRATION  , SOLAR CONSTANTS
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      C       COO=INITIAL GUESS AT RHO-PLUS AT ZERO
      C           WHICH IS SQUARE OF (COO*R1)
      C       R1= REFLECTIVITY AT LEFT END
      C       R2= REFLECTIVITY AT RIGHT END
      C      ZE=DISTANCE FOR LIGHT INTENSITY TO DIMINISH BY FACTOR 1/E
      C       TM= TRANSMISSION COEFFICIENT (OUTPUT MIRROR)
      C      ZOL=POINT ALONG AXIS WHERE MAXIMUM ILLUMINATION OCCURS
      C     IN THE CASE ILLUMINATION IS A BELL SHAPED CURVE
      C      IN THE CASE OF A SQUARE WAVE, 2*ZOL IS CUT OFF POINT
      C        THE POINT 2*ZOL IS WHERE ILLUMINATION BEGINS TO DIMINISH
      C      LC=LENGTH OF CAVITY
      C     ZL=2*ZOL    LENGTH WHICH IS ILLUMINATED
      C      FRAC=FRACTION OF PEAK CONCENTRATION WHICH GOES
      C           INTO HEAT
      C          DEFAULT VALUEE IS FRAC=0.184 I.E. 1.84 PERCENT
      C
      601    CONTINUE
             P=PTO
             TO=T
             ETAO=P*(1.01325E5)*296./(8317.*760.*T)
      C      ETAO IN KG/M**3
      C      P IN TORR
      C      T IN DEG K
             CMIN=1.0E10
             CMAX=1.0E30
            ZL=2*ZOL
             L=LC
             CO=CON
             C11=CON
            CALL COEFFS
      C      WO IN M/SEC
             WO=OMEGA/100.
      C      OMEGA AND OMEGA ARE IN CM/SEC
             WRITE(6,198)
      198    FORMAT(///)
            WRITE(6,199)  ZE,ZOL,CON,OMEGA,COO,R1,R2,P,T
      199    FORMAT(1X, T5,5HZE = ,F10.3,T30,6HZOL = ,E15.7,T55,6HCON = ,
           1 E15.7,T80,8HOMEGA = ,E15.7,/,
           2 1X,T5,6HCOO = ,E15.7, T30,6H R1 = ,F10.7, T55,6H R2 = ,F10.7,
           3 T80,4H P = ,E15.7 ,T105,7HTEMP =  ,F10.3)
      C     SET UP COEFFICIENTS IN DIFFERENTIAL EQUATIONS
      C       SET PRINTER OFF
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                C       IPRINT=0        PRINTER OFF
                C       IPRINT=1        PRINTER ON
                      IPRINT=0
      130             C       SET STEP SIZE H=1.0 CM
                      H=1.0
                C     INTEGRATE DIFFERENTIAL EQUATIONS FROM Z=0 TO Z=LC
                      X1=COO
                      CALL INTEG(IPRINT,H)
      135             C
                C       INTERVAL HALVING SCHEME
                C
                C      W1 AND W2 ARE WEIGHTS FOR INTERVAL HALVING SCHEME FOR
                C      DETERMINING COO WHICH SATISFIES BOUNDARY CONDITIONS
      140           Y1=ABC
                     IF(Y1.LT.0) PER=.1
                CC     IF(Y1.LT.0) PER=.9
                     IF(Y1.GT.0) PER=10.
                CC     IF(Y1.GT.0) PER=1.1
      145       702  CONTINUE
                     COO=(PER)*COO
                     IF(COO .LT. CMIN) STOP 5432
                     IF(COO .GT. CMAX) STOP 2345
                    X2=COO
      150           CALL INTEG(IPRINT,H)
                    Y2=ABC
                     IF((Y1*Y2).LT. 0)GO  TO 701
                     X1=COO
                     Y1=Y2
      155            GO TO 702
                701  CONTINUE
                     W1=.4
                     W2=.6
                    COO=W2*X1+W1*X2
      160       708  CONTINUE
                     CALL INTEG(IPRINT,H)
                     X3=COO
                     Y3=ABC
                     IF(ABS(Y3).LT.0.001) GO TO 555
      165       704  CONTINUE
                     IF((Y1*Y3).LT. 0) GO TO 705
                C    Y1 & Y3 ARE OF THE SAME SIGN
                     X1=X3
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```
                      Y1=Y3
170                   W3=ABS(2*Y1)+ABS(Y2)
                      W1=ABS(2*Y1)/W3
                      W2=ABS(Y2)/W3
                      COO=W2*X1+W1*X2
                      GO TO 708
175             705   CONTINUE
                C     Y1 & Y3 ARE OF OPPOSITE SIGN
                      X2=X3
                      Y2=Y3
                      W3=ABS(2*Y1)+ABS(Y2)
180                   W1=ABS(2*Y1)/W3
                      W2=ABS(Y2)/W3
                      COO=W2*X1+W1*X2
                      GO TO 708
                555    IPRINT=1
185                    H=0.25
                       CALL INTEG(IPRINT,H)
                       GO TO 55
                     END
```

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```
      SUBROUTINE GRAPHS(JJJ)
      COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
      COMMON/BLK8/ZUL,ZE,NG,TO,RAD,A
      COMMON/BLK30/DATA(1352,50),NDMAX,FLRATE(8)
      DIMENSION X(1352),Y(1352),YY(1352,8)
      REAL LC
C     JJJ=1,5
C     JJJ=1 PLOT R VS Z
C     JJJ=2 PLOT I2 VS Z
C     JJJ=3 PLOT I* VS Z
C     JJJ=4 PLOT I VS Z
C     JJJ=5 PLOT INV VS Z
C
C     DATA ARRAY IS BY COLUMNS
C     Z,R,I2,I*,I,INV,Z,R,I2,I*,I,INV,...
C     ND=NUMBER OF DATA POINTS,=NUMBER OF ROWS IN DATA ARRAY
C     NG=NUMBER OF CURVES PER GRAPH
C     IC IS CODE TO DETERMINE NUMBER OF GRAPHS TO PLOT
C     IC=0 FOR MORE THAN ONE GRAPH
C     IC=1 FOR LAST GRAPH (USED FOR ONLY ONE GRAPH)
C
      IC=0
      NLAST=NG-1
      IF(NLAST .EQ. 0) IC=1
C     PLOT JJJ VS Z
      DO 10 I=1,NDMAX
      X(I)=DATA(I,1)
      DO 20 J=1,NG
      NN=(J-1)*6
      NCOL=NN+1+JJJ
      YY(I,J)=DATA(I,NCOL)
20    CONTINUE
10    CONTINUE
C     FIND YMAX,YMIN
      DMAX=0.0
      YMAX=20.0
      YMIN=0.0
      ZMIN=0.0
C     PLOT FIRST DATA CURVE
C     JJJ=1
      BB=LC/10.
      IBB=1+INT(BB)
```

ORIGINAL PAGE IS
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```
                ZMAX=10.*IBB
                 DO 40 I=1,NDMAX
45              IF(ABS(YY(I,1)).LE. 1.0) GO TO 41
                Y(I)=(ALOG10(ABS(YY(I,1))) )*SIGN(1.0,YY(I,1))
                GO TO 40
           41   Y(I)=0.0
           40   CONTINUE
50              ZMIN=0.0
                IF(JJJ.GT.1) GO TO 50
           C    JJJ=1   PLOT R VS Z
                CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
               1  22,22HZ, AXIAL DISTANCE, CM    ,
55             2  11,11HLOG (C3F7) ,0,
               3  10.,4.,1.5,1.5)
                GO TO 600
           50   CONTINUE
                IF(JJJ.GT.2) GO TO 100
60         C    JJJ=2   PLOT I2 VS Z
                CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
               1  23,23HZ, AXIAL DISTANCE, CM   ,
               2  9,9HLOG (I2)  ,0.,
               3  10.,4.,1.5,1.5)
65              GO TO 600
          100   CONTINUE
                IF(JJJ.GT.3) GO TO 200
           C    JJJ=3   PLOT I* VS Z
                CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
70             1 23,23HZ, AXIAL DISTANCE, CM  ,
               2  9,9HLOG (I*)  ,0,
               3  10.,4.,1.5,1.5)
                GO TO 600
          200   CONTINUE
75              IF(JJJ.GT.4) GO TO 300
           C    JJJ=4    PLOT  I VS Z
                CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
               1  23,23HZ, AXIAL DISTANCE, CM  ,
               2  8,8HLOG (I)  ,0,
80             3  10.,4.,1.5,1.5)
                GO TO 600
          300   CONTINUE
                YMIN=-20.0
           C    JJJ=5   PLOT 1NV VS Z
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
     1  23,23HZ, AXIAL DISTANCE, CM  ,
     2  24,24H+,-LOG(ABS([I*]-.5*[I])) ,0,
     3  10.,4.0,1.5,1.5)
  600 CONTINUE
C     PLOT REST OF CURVES OR EXIT IF ONLY ONE CURVE
      NLAST=NG-1
      IF(NLAST .EQ. 0) GO TO 601
      DO 500  J=2,NLAST
      DO 501 I=1,NDMAX
      IF(ABS(YY(I,J)) .LE. 1.0) GO TO 502
      Y(I)=(ALOG10(ABS(YY(I,J))) )*SIGN(1.0,YY(I,J))
      GO TO 501
  502 Y(I)=0.0
  501 CONTINUE
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
     1  1,1H   ,1,1H    , 0.,10.,4.,1.5,1.5)
  500 CONTINUE
C     PLOT LAST CURVE
      DO 60 I=1,NDMAX
      IF(ABS(YY(I,NG)) .LE. 1.0) GO TO 61
      Y(I)=(ALOG10(ABS(YY(I,NG))) )*SIGN(1.0,YY(I,NG))
      GO TO 60
   61 Y(I)=0.0
   60 CONTINUE
      CALL INFOPLT(1,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
     1 1,1H  ,1,1H  ,0.,10.,4.,1.5,1.5)
  601    CONTINUE
      CALL NFRAME
      RETURN
      END
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
      SUBROUTINE PFLOW
C     SUBROUTINE TO CALCULATE THE PARAMETERS FOR SUBROUTINE FLOW
C     PARAMETERS STORE IN COMMON BLK10
      COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
      COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
      COMMON/BLK10/CF1,CF2,CF4,QF0,RSTAR,ZL,L,SF1,SF2,AR,AA0,BB0
      COMMON/BLK23/W0,ETA0,PT0,FRAC
      REAL L
C
C     AR IS BEAM DIAMETER RADIUS IN CM
      SF1=1000./296.
      SF2=(1.01325E5)/760.
C     SF1,SF2 ARE SCALE FACTORS FOR THE CORRECT UNITS OF
C     P=PRESSURE (N/M**2) , SF1 (MOLE/KG)
C     PT=PRESSURE (TORR),  SF2 (N/M**2)/TORR
C     ZL=LIGHT SOURCE LENGTH IN CM
C     ETA=DENSITY (KG/M**3)
C     L=TUBE LENGTH IN CM
C     RSTAR=GAS CONSTANT (JOULE/KG DEG K)
C     T=TEMPERATURE (DEG K)
C     CV=SPECIFIC HEAT AT CONSTANT VOLUME
C     W=FLOW VELOCITY (M/SEC) (SUBSCRIPTS 0,L FOR START,END)
      P0=SF2*PT0
      RSTAR=6317.0/296.0
      CF1=ETA0*W0
      CF2=CF1*W0+P0
C     INTEGRAL OF CV(T)DT IS GIVEN BY
      XXX=BB0*(T0-300)
      CALL ETO(XXX,YYY)
      CVINT0=SF1*(AA0/BB0)*YYY
C     CONSTANTS CF4 AND QF0
      CF4=CF1*(RSTAR*T0+CVINT0)+CF1*W0*W0*.5
      QF0=FRAC*(1.35E3)*C0
      QF0=QF0*1.0/ZL
      RETURN
      END
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
      SUBROUTINE FLOW(Z,T,PTORR,W,ETA)
      COMMON/BLK8/ZDL,ZE,NG,TO,RAD,A
C     SUBROUTINE TO CALCULATE T,P,W,ETA AS FUNCTION OF Z
      COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AAO,BBO
      COMMON/BLK23/WO,ETAO,PTO,FRAC
C
      COMMON/BLK29/ ZZZ,TZZ,PZZ,ETAZZ,WZZ
      REAL L
      ICOUNT=0
      Q=QFO*Z
C     ENERGY INPUT TERM DETERMINED BY QFO
      IF(Z.GT.ZL)    Q=QFO*ZL
      T=TO
50    CONTINUE
      W=(CF2-SQRT(CF2*CF2-4.*CF1*CF1*RSTAR*T))/(2.*CF1)
      ETA=CF1/W
      XXX=BBO*(T-300)
      CALL ETO(XXX,YYY)
      P=ETA*RSTAR*T
      F=CF1*RSTAR*T+CF1*SF1*(AAO/BBO)*YYY+CF1*.5*W*W-Q-CF4
      FP=CF1*RSTAR+CF1*SF1*AAO*YYY+W*(ETA*RSTAR)/((P/W)-CF1)
      T1=T-F/FP
      ERROR=ABS(100*(T1-T)/T)
      IF(ERROR .LT. 1.0) GO TO 100
      T=T1
      ICOUNT=ICOUNT+1
      IF(ICOUNT .GT. 100) STOP 4444
      GO TO 50
100   CONTINUE
      T=T1
      W=(CF2-SQRT(CF2*CF2-4.*CF1*CF1*RSTAR*T))/(2.*CF1)
      TC=T-273
      ETA=CF1/W
      PNM2=ETA*RSTAR*T
      PTORR=PNM2/SF2
      ZZZ=Z
      TZZ=TC
      PZZ=PTORR
      ETAZZ=ETA
      WZZ=W
      RETURN
      END
```

ORIGINAL PAGE IS
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```
      SUBROUTINE ARREN(TEMP)
C     SUBROUTINE FOR ARRENHIUS EXPRESSION OF RATE COEFFICIENTS
C     BASIC ASSUMPTIONS
C      FOR QI TERMS QI=QIO*EXP(-BETA*(TEMP-TO))
C      TREAT KI TERMS LIKE CI TERMS
C
      COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
      COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
      COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
      COMMON/BLK11/KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
      COMMON/BLK12/QQ1,QQ2,QQ3,QQ4,QQ5
      COMMON/BLK13/CC1,CC2,CC3,CC4,CC5,CC6
      REAL K1,K2,K3,K4,K5,K6,K7,K8,KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
C
C     REFERENCE J.S. COHEN AND O.P. JUDD
C                J.APPL. PHYS., VOL 55, NO. 7, APRIL 1984
C     COEFFICIENTS MODIFIED TO ACHIEVE SPECIFIC VALUES AT TEMPERATURE
C     OF 276 DEGREES K.
C
      BETA=4.4E-3
      SF1=1.0
      XXX=-BETA*(TEMP-300)
      CALL ETO(XXX,YYY)
      SF2=YYY
      K1=KK1*SF1
      K2=KK2*SF1
      K3=KK3*SF1
      K4=KK4*SF1
      K5=KK5*SF1
      K6=KK6*SF1
      K7=KK7*SF1
      K8=KK8*SF1
      C1=CC1*SF1
      C2=CC2*EXP(1205.76/TEMP)
      C3=CC3*SF1
      XYZ=-29.5207-5.844*ALOG(TEMP/300.)+2.163*(ALOG(TEMP/300.))**2
      C4=10.0**XYZ
      C5=CC5*EXP(1191.626/TEMP)
      C6=CC6*SF1
      Q1=QQ1*SF1
      Q2=QQ2*EXP(-4.4E-3*(TEMP-300))
      Q3=QQ3*SF1
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
                Q4=Q04*SF1
                Q5=Q05*SF1
45              RETURN
                END
```



```
 1              FUNCTION CHSI1(Z)
              C IMPLICIT REAL*8(A-H,K,L,O-Z)
                COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
                COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
 5              REAL LC
                IF(Z.LT.ABARO) GO TO 100
                IF(Z.LT.Z1BAR) GO TO 200
              C Z GREATER THAN Z1BAR
              100 CHSI1=0.0
10            C  CHSI1 HAS UNITS OF SEC^-1
                RETURN
              200 CONTINUE
                CHSI1=CHSI10
                RETURN
15              END
```



```
 1              SUBROUTINE ETO(X,Y)
                IF(X .LT. -670.) GO TO 100
                Y=EXP(X)
                RETURN
 5            100 Y=0.
                RETURN
                END
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
FUNCTION CHSI2      74/860  OPT=1  PMDMP          FTN 4.8+688      88/11/02. 14.55.42      PAGE     1

      C
            FUNCTION CHSI2(Z)
      C     IMPLICIT REAL*8(A-H,K,L,O-Z)
            COMMON/BLK4/CHSI1O,CHSI2O,ABARO,Z1BAR,LC
            COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
            REAL LC
            IF(Z.LT.ABARO) GO TO 100
            IF(Z.LT.Z1BAR) GO TO 200
      C     Z GREATER THAN Z1BAR
             XXX=-(Z-Z1BAR)/ZE
             CALL ETO(XXX,YYY)
            CHSI2=CHSI2O*YYY
      C     CHSI2 HAS UNITS OF SEC^-1
            RETURN
      100   CHSI2=0.0
            RETURN
      200   CONTINUE
            CHSI2=CHSI2O
            RETURN
            END
```

```
SUBROUTINE VELOC    74/860  OPT=1  PMDMP          FTN 4.8+688      88/11/02. 14.55.42      PAGE     1

      C
            SUBROUTINE VELOC(OMEG1,RAD,OMEGA,A)
      C     CALCULATE VELOCITY OMEGA AT R=RAD
      C          0 .LE. RAD  .LE. A
      C
      C     TYPE OF FLOW
            OMEGA=(OMEG1/(A*A))*(RAD-A)**2
            RETURN
            END
```

ORIGINAL PAGE IS
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```
      C
            SUBROUTINE COEFFS
      C       THIS SUBROUTINE DEFINES THE COEFFICIENTS IN THE DIFFERENTIAL
      C       EQUATIONS TO BE SOLVED.
      C     IMPLICIT REAL*8(A-H,K,L,O-Z)
            COMMON/BLK22/AD,V1,V2,GG
            COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
            COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
            COMMON/BLK7/ABC,C00,CO,OMEG1,P,R1,R2,TM,XNRHO
             COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
             COMMON/BLK11/KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
             COMMON/BLK12/QQ1,QQ2,QQ3,QQ4,QQ5
            COMMON/BLK13/CC1,CC2,CC3,CC4,CC5,CC6
            REAL KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8,LC
      C
      C     COEFFICIENTS IN THE DIFFERENTIAL EQUATIONS
      C
            OMEGA=OMEG1
             CALL VELOC(OMEG1,RAD,OMEGA,A)
            ABARO=0.0
      C      ABARO= START OF ILLUMINATION
      C        Z1BAR=2*ZOL = POINT ON AXIS WHERE ILLUMINATION BEGINS TO DIMINISH
            CHSI10=(3.04E-3)*CO*XNRHO
      C        C00 IS THE CONCENTRATION IF SOLAR CONSTANTS
            CHSI20=(3.38E-2)*CO
            Z1BAR=2*ZOL
            EPSNU=1.5E-19
      C      WATTS*SEC
            A00=2.0E17
            B00=.443
      C
      CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      C
      C        (CHSI1)    HV + R1 --> R + I*
      C        (CHSI2)    HV + I2 --> I* + I    (51% OF THE TIME)
      C        (CHSI2)    HV + I2 -->  1 + I    (49% OF THE TIME)
      CC          (KK1)      I* + R --> R1
      CC          (KK2)      I + R --> R1
      CC          (KK3)      R + R --> P2
      CC          (KK4)      R + R1 --> R2 + I
      CC          (KK5)      R + I2 --> R1 + 1
      CC          (KK6)      R + R1 --> R2 + I*
```

ORIGINAL PAGE IS
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```
      CC          (KK7)     I* + RI --> I2 + R
      CC          (KK8)     I + RI --> I2 + R
45    CC
      CC          (001)     I* + RI --> I + RI
      CC          (002)     I* + I2 --> I + I2
      CC          (003)     I* + R --> I + R
      CC          (004)     I* + R2 --> I + R2
50    CC          (005)     I* + I --> I + I
      CC
      CC          (CC1)     I* + I + RI --> I2 + R1
      CC          (CC2)     I + I + RI --> I2 + R1
      CC          (CC3)     I* + I + I2 --> I2 + I2
55    CC          (CC4)     I + I + I2 --> I2 + I2
      CC          (CC5)     I + I + R2 --> I2 + R2
      CC          (CC6)     I + I* + R2 --> I2 + R2
      CC
      CC
60    CC        WALL REACCTIONS
      CC
      CC         (V1)     I + I + WALL --> I2 + WALL
      CC         (V2)    R2 + I + WALL --> R + RI + WALL
      CC
65    CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      CC
      CC      KK1 = 34.7E-13
      CC      KK1 = 5.6E-13
            KK1 = .9E-13
70    CC
            KK2 = 8.05E-11
      CC      KK2 = 2.3E-11
      CC      KK2 = .657E-11
      CC
75    CC      KK3 = 10.4E-12
      CC      KK3 = 2.6E-12
            KK3 = .26E-11
      CC
      CC      KK4 =     9.E-16
80    CC      KK4 = 3.E-16
            KK4 =      1.E-16
      CC
            KK5 =     3.E-11
      CC      KK5 = 1.0E-11
```

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```
      CC     KK5 =      .33E-11
      CC
            KK6 = 10.24E-17
      CC     KK6 = 3.2E-17
      CC     KK6 = 1.E-17
      CC
      CC     KK7 = 4.5E-19
      CC     KK7 = 3.0E-19
            KK7 = 1.5E-19
      CC
      CC     KK8 =       4.8E-23
      CC     KK8 = 1.6E-23
      CC     KK8 =       .53E-23
            KK8 = 0.0
      CC
      CC     QQ1 = 8.4E-16
      CC     QQ1 = 2.0E-16
            QQ1 = .476E-16
      CC
      CC     QQ2 = 4.94E-11
      CC     QQ2 = 1.9E-11
            QQ2 = .65868E-11
      CC
      CC     QQ3 =       11.1E-18
      CC     QQ3 = 3.7E-18
            QQ3 =      1.23E-18
      CC
      CC     QQ4 =      14.1E-16
      CC     QQ4 = 4.7E-16
            QQ4 =      1.57E-16
      CC
      CC     QQ5 =      4.8E-14
      CC     QQ5 = 1.6E-14
            QQ5 =      .53E-14
      CC
      CC     CC1 = 10.2E-33
      CC     CC1 = 3.2E-33
            CC1 = 1.E-33
      CC
            CC2 = 5.7E-33
      CC     CC2 = 8.5E-32
      CC     CC2 = 1.6E-32
```

ORIGINAL PAGE IS
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```
                CC
                CC      CC3 = 14.4E-32
                CC      CC3 = 8.E-32
      130       C       CC3 = 4.44E-32
                CC
                C       CC4 = 4.94E-30
                CC      CC4 = 3.8E-30
                CC      CC4 = 2.92E-30
      135       CC
                CC      CC5 = 6.E-31
                C       CC5 = 8.0E-33
                CC      CC5 = 3.6E-31
                CC
      140       CC      CC6 =       2.25E-32
                CC      CC6 =       1.8E-32
                CC      CC6 =       1.35E-32
                C       CC6 = 0.0
                CC
      145       C       V1 =        3.0E-12
                C       V1 =        1.0E-12
                C       V1 =        .33E-12
                C       V1 = 0.0
                C
      150       C       V2 =        3.0E-11
                C       V2 =        1.0E-11
                C       V2 =         .33E-11
                C       V2 = 0.0
                C
      155       CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
                C
                C       KK1=.903E-13
                C       KK2=80.E-12
                C       KK3=.65E-12
      160       C       KK4=1.000E-16
                C       KK5=3.009E-11
                C       KK6=1.0E-17
                C       KK7=.1517E-18
                C       KK8=1.6E-23
      165       C
                C       Q01=.476E-16
                C       Q02=1.9E-11
                C       Q03=.1235E-17
```

ORIGINAL PAGE IS
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```
C     Q04=1.57E-16
C     Q05=.53E-14
C
CC     CC1=1.053E-33
CC     CC2=45.0E-32
CC     CC3=.4447E-31
CC     CC4=4.94E-30
CC     CC5=3.6E-31
CC     CC6=      1.8E-32
C
C     V1=       1.0E-12
C     V2=       1.0E-11
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      GG=2*(.18/LC)**2
      C=3.0E10
      B=(9.66E18)*P/T0
      B2=B*B
      B3=B2*B
CC       WRITE OUT CCOEFFICCIENTS
      WRITE(6,100) KK1,KK7,QQ1,CC5
      WRITE(6,101) KK2,KK8,QQ2,V1
      WRITE(6,102) KK3,CC1,QQ3,V2
      WRITE(6,103) KK4,CC2,QQ4,RAD
      WRITE(6,104) KK5,CC3,QQ5,A
      WRITE(6,105) KK6,CC4,CC6
100   FORMAT(T5,5HKK1 = ,E15.7,T30,5HKK7 = ,E15.7,T60,5HQQ1 = ,E15.7 ,
     1 T85,5HCC5 =  , E15.7 )
101   FORMAT(T5,5HKK2 = ,E15.7,T30,5HKK8 = ,E15.7,T60,5HQQ2 = ,E15.7 ,
     1 T85,5HV1 =  , E15.7 )
102   FORMAT(T5,5HKK3 = ,E15.7,T30,5HCC1 = ,E15.7,T60,5HQQ3 = ,E15.7 ,
     1  T85, 5HV2 =  , E15.7)
103   FORMAT(T5,5HKK4 = ,E15.7,T30,5HCC2 = ,E15.7,T60,5HQQ4 = ,E15.7,
     1 T85, 6HRAD = ,F10.4 )
104   FORMAT(T5,5HKK5 = ,E15.7,T30,5HCC3= ,E15.7,T60,5HQQ5 = ,E15.7,
     1 T85, 6H A  =  ,F10.4 )
105   FORMAT(T5,5HKK6 = ,E15.7,T30,5HCC4= ,E15.7,T60,5HCC6 = ,E15.7 )
      RETURN
      END
```

ORIGINAL PAGE IS
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```
      SUBROUTINE FUN(N,Z,Y,F)
C       THIS SUBROUTINE DEFINES THE RIGHT HAND SIDE
C       OF THE DIFFERENTIAL EQUATIONS FOR THE CHEMICAL KINETICS
C     IMPLICIT REAL*8(A-H,K,L,O-Z)
      DIMENSION Y(7),F(7)
      COMMON/BLK1/X7,POWER
      EXTERNAL CHSI1,CHSI2
      COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
      COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
      COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
      COMMON/BLK4/CHSI10,CHSI20,ABAR0,Z1BAR,LC
      COMMON/BLK7/ABC,C00,C0,OMEG1,P,K1,K2,TM,XNRHO
      COMMON/BLK22/AD,V1,V2,GG
      REAL K1,K2,K3,K4,K5,K6,K7,K8,LC
C
C     QY=QUANTUM YIELD
      QY=1.0
C
C       F(I),I=1,6 ARE RATES OF CHANGES FOR THE CONCENTRATIONS
C         F(1)=D[R1]/DZ                F(2)=D[R]/DZ
C         F(3)=D[R2]/DZ                F(4)=D[I2]/DZ
C         F(5)=D[I*]/DZ                F(6)=D[I]/DZ
C
   20 CONTINUE
C      Z IS DISTANCE IN CM
C      CALCULATE GAS PARAMETERS AS FUNCTION OF Z
C      CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY)
       CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY)
C      TEMP IS TEMPERATURE DEG K
C      PRESS IS PRESSURE IN TORR
C      FLOWR IS FLOWRATE IN M/SEC
C      DENSITY IS GAS DENSITY IN KG/M**3
       OMEGA=FLOWR*100.
C      OMEGA IS FLOW RATE IN CM/SEC
C      CALCULATE COEFFICIENTS AS FUNCTION OF TEMP AND Z
       CALL ARREN(TEMP)
C      CONSTANTS COME VIA COMMON BLKS 2 AND 3
C      K'S IN CM**3/SEC
C      C'S IN CM**6/SEC
C      Q'S IN CM**3/SEC
C      POWER IS IN W/CM**2
       X8=C00/(Y(7)*B)
```

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```
      X7STAR=Y(7)*B+X6
      DIF=Y(5)-.5*Y(6)
      CALL SIGMA(SIG2)
      SIG=SIG2
     F(1)=K1*B*Y(2)*Y(5)+K2*B*Y(2)*Y(6)-CHSI1(Z)*Y(1)-K4*B*Y(1)*Y(2)
    1 +K5*B*Y(2)*Y(4) -K7*B*Y(5)*Y(1)-K6*B*Y(2)*Y(1)  +V2*B*Y(3)*Y(6)
    2  -K8*B*Y(6)*Y(1)
     F(2)=CHSI1(Z)*Y(1)-K1*B*Y(2)*Y(5)-K2*B*Y(2)*Y(6)-2*K3*B*Y(2)*Y(2)
    1 -K4*B*Y(1)*Y(2)-K6*B*Y(1)*Y(2)-K5*B*Y(2)*Y(4)+V2*B*Y(3)*Y(6)
    2 +K7*B*Y(5)*Y(1) +K8*B*Y(6)*Y(1)
     F(3)=K3*B*Y(2)*Y(2)+K6*B*Y(1)*Y(2)+K4*B*Y(1)*Y(2)-V2*B*Y(3)*Y(6)
     A1=C1*B2*Y(1)*Y(5)*Y(6)+C2*B2*Y(1)*Y(6)*Y(6)+C3*B2*Y(4)*Y(5)*Y(6)
     A2=C4*B2*Y(4)*Y(6)*Y(6)-CHSI2(Z)*Y(4)+K7*B*Y(5)*Y(1)
    1 -K5*B*Y(2)*Y(4) +V1*B*Y(6)*Y(6) +C5*B2*Y(6)*Y(6)*Y(3)
     F(4)=A1+A2 +K8*B*Y(6)*Y(1) +C6*B2*Y(6)*Y(5)*Y(3)
     A3=QY*CHSI1(Z)*Y(1)+0.51*CHSI2(Z)*Y(4)-K1*B*Y(2)*Y(5)
     A4=-C1*B2*Y(1)*Y(5)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)-Q1*B*Y(1)*Y(5)
     A5=-Q2*B*Y(4)*Y(5)-C*SIG*X7STAR*DIF +K6*B*Y(2)*Y(1)
     F(5)=A3+A4+A5-Q3*B*Y(5)*Y(2)-Q4*B*Y(5)*Y(3)-Q5*B*Y(5)*Y(6)
    1 -K7*B*Y(5)*Y(1)  -C6*B2*Y(6)*Y(5)*Y(3)
     A6=1.49*CHSI2(Z)*Y(4)+Q1*B*Y(1)*Y(5)+Q2*B*Y(4)*Y(5)
    1  -2*C5*B2*Y(6)*Y(6)*Y(3)  -K8*B*Y(6)*Y(1)
     A7=C*SIG*X7STAR*DIF -C1*B2*Y(1)*Y(5)*Y(6)
     A8=-2*C2*B2*Y(1)*Y(6)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)
     A9=-2*C4*B2*Y(4)*Y(6)*Y(6)-K2*B*Y(2)*Y(6)+K4*B*Y(1)*Y(2)
      A10=Q3*B*Y(5)*Y(2)+Q4*B*Y(5)*Y(3)+Q5*B*Y(5)*Y(6)
    1 +K5*B*Y(2)*Y(4)  -V2*B*Y(3)*Y(6) -2*V1*B*Y(6)*Y(6)
     F(6)=A6+A7+A8+A9+A10 -C6*B2*Y(6)*Y(5)*Y(3)
     DO 10 I=1,6
  10 F(I)=F(I)/OMEGA
      F(7)=Y(7)*DIF*B*SIG
     RETURN
     END
```

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```
      C
            SUBROUTINE SIGMA(SIG)
      C     THIS SUBROUTINE DEFINES THE CROSS SECTION SIGMA
           COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
           COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
            REAL NU,NUS,NU0,NU1,NU2,NU3,NU4 ,NU5
            PI=3.14159
            PIS=PI*PI
            NU=C/1.315246E-4
            NUS=NU*NU
            PISNUS=PIS*NUS*4.
            G=0
            CS=C*C
            NU0=NU
            NU1=NU0+.141*C
            NU2=NU1+.068*C
            NU3=NU0-.427*C
            NU4=NU3-.026*C
            NU5=NU4-.068*C
            DELTA23=NU-NU5
            DELTA22=NU-NU4
            DELTA21=NU-NU3
            DELTA34=NU-NU0
            DELTA33=NU-NU1
            DELTA32=NU-NU2
            TEMP0=293
            TWALL=TEMP0
            T1=TWALL
            A=5.434
            A1=A*2.4/7.7*CS
            A2=A*3.0/7.7*CS
            A3=A*2.3/7.7*CS
            A4=A*5.0/7.7*CS
            A5=A*2.2/7.7*CS
            A6=A*0.6/7.7*CS
            FUGTEMP=SQRT(T1/300.)
            ALPHAM=1.88E7*FUGTEMP
            DELDOP=2.51E8*FUGTEMP
            DELNU=DELDOP+ALPHAM*P
            SIGMA23=A1/(PISNUS*DELNU)/(1+(2.*DELTA23/DELNU)**2)*5./12.
            SIGMA22=A2/(PISNUS*DELNU)/(1+(2.*DELTA22/DELNU)**2)*5./12.
            SIGMA21=A3/(PISNUS*DELNU)/(1+(2.*DELTA21/DELNU)**2)*5./12.
```



```
            SIGMA34=A4/(PISNUS*DELNU)/(1+(2.*DELTA34/DELNU)**2)*7./12.
            SIGMA33=A5/(PISNUS*DELNU)/(1+(2.*DELTA33/DELNU)**2)*7./12.
            SIGMA32=A6/(PISNUS*DELNU)/(1+(2.*DELTA32/DELNU)**2)*7./12.
            SIGMAT=SIGMA23+SIGMA22+SIGMA21+SIGMA34+SIGMA33+SIGMA32
            SIG=SIGMAT
            RETURN
            END
```

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```
      C
            SUBROUTINE INTEG(IPRINT,H)
      C      THIS SUBROUTINE INTEGRATES THE SYSTEM OF DIFFERENTIAL EQUATIONS
      C      USING A VARIABLE STEP SIZE 7TH ORDER RUNGE KUTTA-FEHLBERG METHOD.
      C     IMPLICIT REAL*8(A-H,K,L,O-Z)
            DIMENSION YO(7),X(7),WK(49)
            COMMON/BLK1/X7,POWER
            COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
            COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
            COMMON/BLK7/ABC,COO,CO,OMEG1,P,R1,R2,TM,XNRHO
             COMMON/BLK8/ZUL,ZE,NG,TO,RAD,A
            COMMON/BLK22/AD,V1,V2,GG
            COMMON/BLK29/ZZZ,TZZ,PZZ,ETAZZ,WZZ
            COMMON/BLK30/DATA(1352,50),NDMAX,FLRATE(8)
            EXTERNAL FUN,CHSI1,CHSI2
            REAL LC
      C
      C     INTEGRATE SYSTEM FROM Z=0 TO Z=LC USING RUNGE-KUTTA METHOD
      C
      C     X(1)=RI
      C     X(2)=R
      C     X(3)=R2
      C     X(4)=I2
      C     X(5)=I*
      C     X(6)=I
      C     X(7)=RHO+
      C     X8=RHO-
      C     X9=I*-.5*I
      C
             WW2=(.98)**2
      C     INITIALIZE CONSTANTS FOR FLOW EQUATIONS
      C     SEE COMMON BLK10 FOR THESE CONSTANTS--NEEDED FOR SUB FLOW
            CALL PFLOW
            ND=0
      C       TEST FOR PRINT CONDITIONS
             IF(IPRINT.EQ. 0) GO TO 229
             NG=NG+1
            FLRATE(NG)=OMEGA
             WRITE(8,331) LC
      331    FORMAT(1X,11H   LC    =  ,F10.2)
      229     CONTINUE
      55      CONTINUE
```

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```
      N=7
      TOL=1.0E-6
45    PD=1.0
      MTH=1
C      H IS STEP SIZE IN CM BETWEEN PRINT OUTS
C      IPRINT=0 OFF, IPRINT=1 ON
      HMIN=H/10000000.
50    HMAX=H/100.
      HUSE=HMIN*10
      IERR=0
C     INITIAL CONDITIONS
      Z0=0.0
55    YO(1)=1.0
      Z1=0.0
      DO 9 I=2,6
9     YO(I)=0.0
C       GUESS AT INITIAL CONDITIONS FOR X(7) AND X(8)
60    X70=SQRT(R1*COO)
      YO(7)=X70/B
      IF(IPRINT .EQ. 0) GO TO  300
      WRITE(6,191)
191   FORMAT(///,T7,1HZ,T20,4H[R1],T32,4H[R],T45,5H[R2],T57,4H[I2],
65   1 T69,4H[I*],T80,4H[I] ,T91,6H[RHO+],T103,6H[RHO-],T112,
     2 9HINVERSION       )
300   CONTINUE
C     PRINT OUT
      DO 10 I=1,7
70    10  X(I)=B*YO(I)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       USE CONSERVATION LAWS---THE ABOVE SYSTEM OF DIFFERENTIAL
75    C       EQUATIONS HAS THE TWO INTEGRALS
C
C           [R1] + [R] +2[R2] = CONSTANT= B
C      OR
C            Y(1) + Y(2) + 2Y(3)= 1.0
80    C
C     AND     [R1]  + 2[I2] + [I*] + [I] = B
C       OR
C             Y(1) + 2Y(4) + Y(5) + Y(6) =1.0
C
```

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```
                YOTH2=1.0-YO(1)-2.*YO(3)
                YOTH6=1.0-YO(5)-2.0*YO(4)-YO(1)
      C         TEST TO SEE IF YOTH2 IS ZERO
                ERROR1=0.0
                IF(YOTH2.EQ.0.0 ) GO TO 1555
                ERROR1=(YO(2)-YOTH2)*100/YOTH2
      1555        CONTINUE
                ERROR2=0.0
      C         TEST TO SEE IF YOTH6 IS ZERO
                IF(YOTH6.EQ. 0.0) GO TO 1556
                ERROR2=(YO(6)-YOTH6)*100/YOTH6
      1556        CONTINUE
                IF((ERROR1.OR. ERROR2).GT. .5) WRITE(6,1222)
      1222      FORMAT(1X, 40H ERROR1 OR ERROR2 IS OUT OF BOUNDS       )
      C
      CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      C
      C    END OF TEST FOR CONSERVATION LAWS BEING SATISFIED
      C
      CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
                X8=C00/X(7)
               X9=X(5)-.5*X(6)
                X7STAR=X(7)+X8
      C          USE SUBROUTINE SIGMA TO CALCULATE CROSS SECTION SIGMA
               CALL SIGMA(SIG2)
                IF(IPRINT .EQ. 0) GO TO 222
               WRITE(6,199)ZO,(X(I),I=1,7),X8,X9
      222       CONTINUE
                IF(IPRINT .EQ. 0) GO TO 227
                ICOL=(NG-1)*6
                ND=ND+1
                DATA(ND,ICOL+2)=X(2)
                DATA(ND,ICOL+1)=ZO
                DATA(ND,ICOL+3)=X(4)
                DATA(ND,ICOL+4)=X(5)
                DATA(ND,ICOL+5)=X(6)
                DATA(ND,ICOL+6)=X9
      C         WRITE Z,R,12,I*,1,INV
                WRITE(8,6773) ZO,X(2),X(4),X(5),X(6),X9
      6773      FORMAT(1X,F6.2,2X,5(2X,E15.4))
      227       CONTINUE
               IF(ZO.LE.0.0) GO TO 3567
```

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```
                IF(IPRINT .EQ. 0) GO TO 223
                WRITE(6,303)ZZZ,TZZ,PZZ,ETAZZ,WZZ
          223     CONTINUE
          303   FORMAT(1X,T2,3HZ= ,F5.2,2X,T15,3HT= ,F7.3,2X,T30,
               1 7HPTORR=  ,F9.2,2X,
               2 T55,9HDENSITY = ,F9.6,2X,T80,3HW=  ,F7.2   )
          3567    CONTINUE
          199   FORMAT(1X,E12.5,8E12.5,E12.5 ,E12.5  )
                C
                C       USE 7TH ORDER RUNGE KUTTA INTEGRATION SCHEME WITH VARIABLE STEP
                C       STEP SIZE CAN VARY FROM HMIN TO HMAX
                C       Z0 IS STARTING VALUE FOR Z
                C       Z1 IS NEXT STOPPING POINT IN INTEGRATION SCHEME
                C       TOL IS TOLERENCE
                C       IERR IS ERROR CODE TO DETERMINE IF INTEGRATION WAS SUCCESSFUL
                C      IF INVERSION DENSITY HAS GONE NEG JUMP OUT OF LOOP
                C      IF  (X9.LE.(-.1E-1)) GO TO 111
                C
          100   CONTINUE
                 Z1=Z1+H
                 CALL RKF7(N,Z0,Z1,Y0,TOL,FUN,P0,MTH,HMIN,HMAX,MUSE,WK,IERR)
                 IF(IERR .NE. 0)  WRITE(6,444)
                IF(IERR .NE. 0) STOP 1717
          444   FORMAT(1X,35H IERR IS NOT ZERO                                  )
          200   CONTINUE
                 X(7)=B*Y0(7)
                 X8=C00/X(7)
          60    FORMAT(1X,5(2X,E14.6))
                IF((Z1+.5*H).GE.(LC+.2)) GO TO 111
          CC      IF(X(7) .GT. X8) GO TO 237
                GO TO 300
          500   CONTINUE
                 DO 110 I=1,7
          110    X(I)=B*Y0(I)
                 X8=C00/X(7)
                  X9=X(5)-.5*X(6)
          111     CONTINUE
                  XX7L=B*Y0(7)
                 RHOPL=X70/(SQRT(R2*R1))
                 DO 112 I=1,7
          112    X(I)=B*Y0(I)
                 X8=C00/X(7)
```

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```
                X9=X(5)-.5*X(6)
170             IF(IPRINT .EQ. 0) GO TO 224
               WRITE(6,199)ZG,(X(I),I=1,7),X8,X9
          224   CONTINUE
          C     RHOPL=RHO-PLUS AT Z=L THEORETICAL VALUE
          C     XX7L= CALCULATED VALUE OF RHO-PLUS AT Z=
175       C     ABC =DIFFERENCE=XX7L-RHOPL
               DIF=(((XX7L-RHOPL)/RHOPL)*100)
               ABC=DIF
               IF(IPRINT .EQ. 0) GO TO 225
              WRITE(6,202)DIF,RHOPL,XX7L,COO
180           225   CONTINUE
              202  FORMAT(1X,13HDIFFERENCE = ,E18.9,2X,12HTHEORETICAL=,E18.9,2X,
                  1 10H ACTUAL = , E18.9,2X,6HCOO =    ,E18.8 )
              237   CONTINUE
              C
185           XX7L=X(7)
              CC    TM=1-R2/(WW2)
              CC    IF(TM .LT. 0) GO TO 300
               POWER=EPSNU*TK*C*XX7L
               IF(IPRINT .EQ. 0) GO TO 226
190            WRITE(6,193)R1,R2,POWER,TM,ZO,P
              226   CONTINUE
              193  FORMAT(1X,5HR1 = ,F10.7,1X,5HR2 = ,F10.7,1X,7HPOWER = ,E18.10,
                  1 1X,5HTM = ,F10.8,1X,4HL = ,F15.7 ,2X,4HP = ,F15.7 )
               IF((Z1+.5*H).GE.(LC+.2)) GO TO 501
195            GO TO 300
              501   CONTINUE
               NDMAX=ND
              RETURN
              END
```

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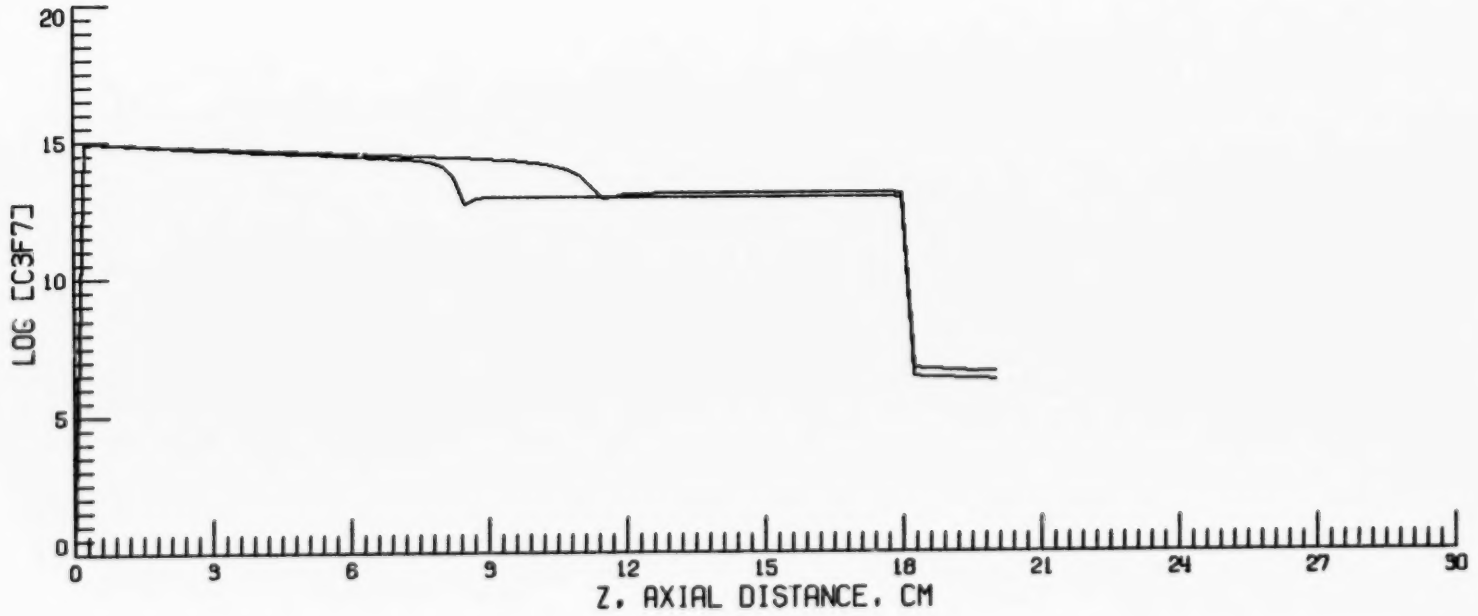
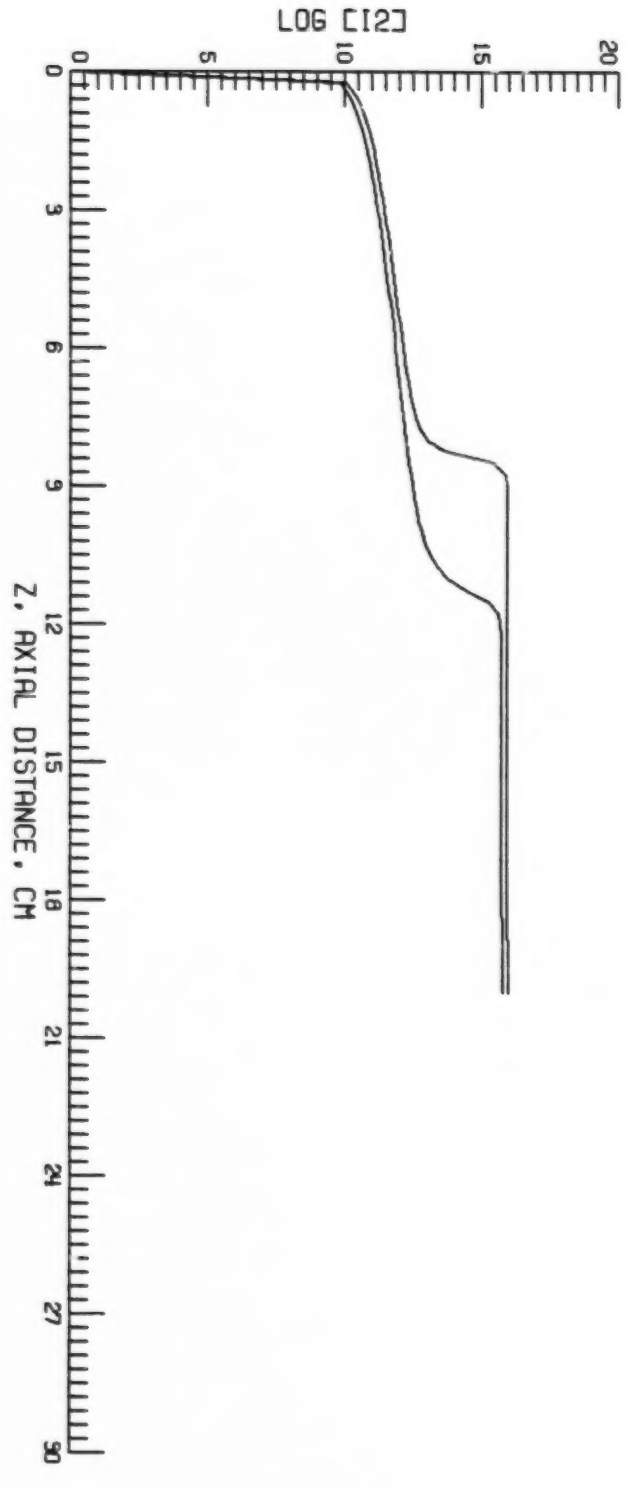
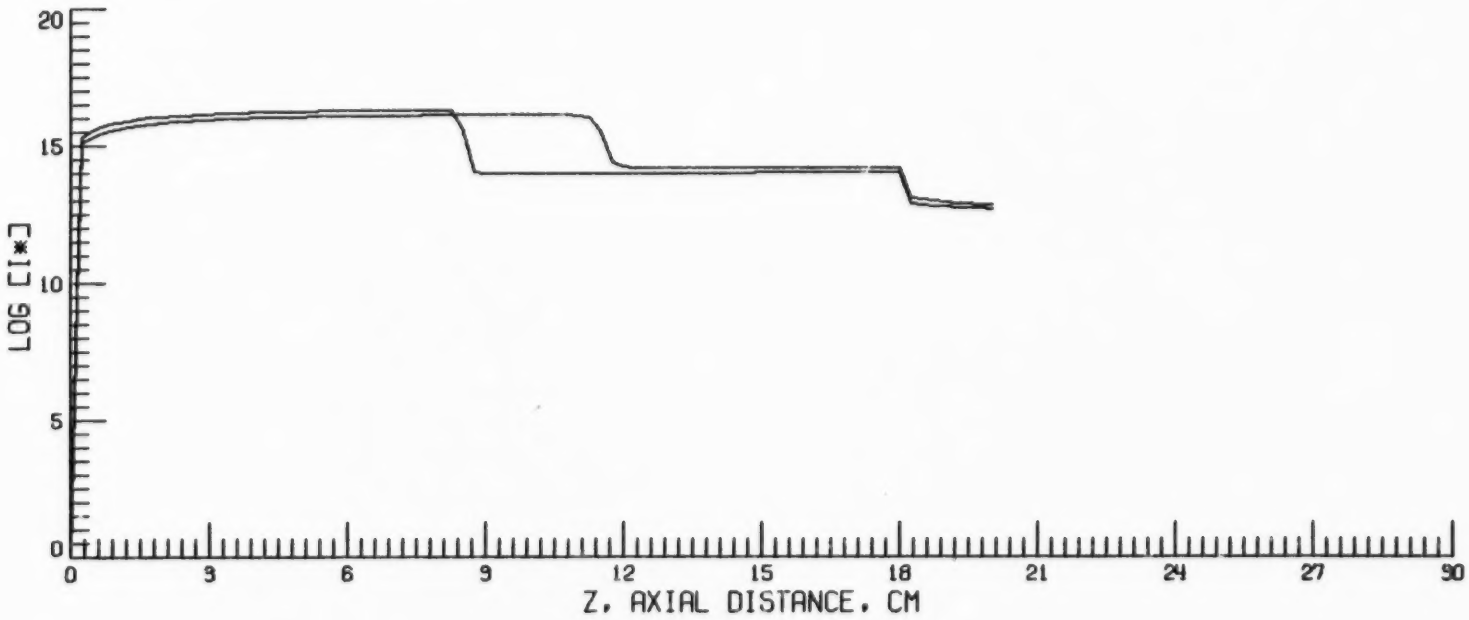
APPENDIX B



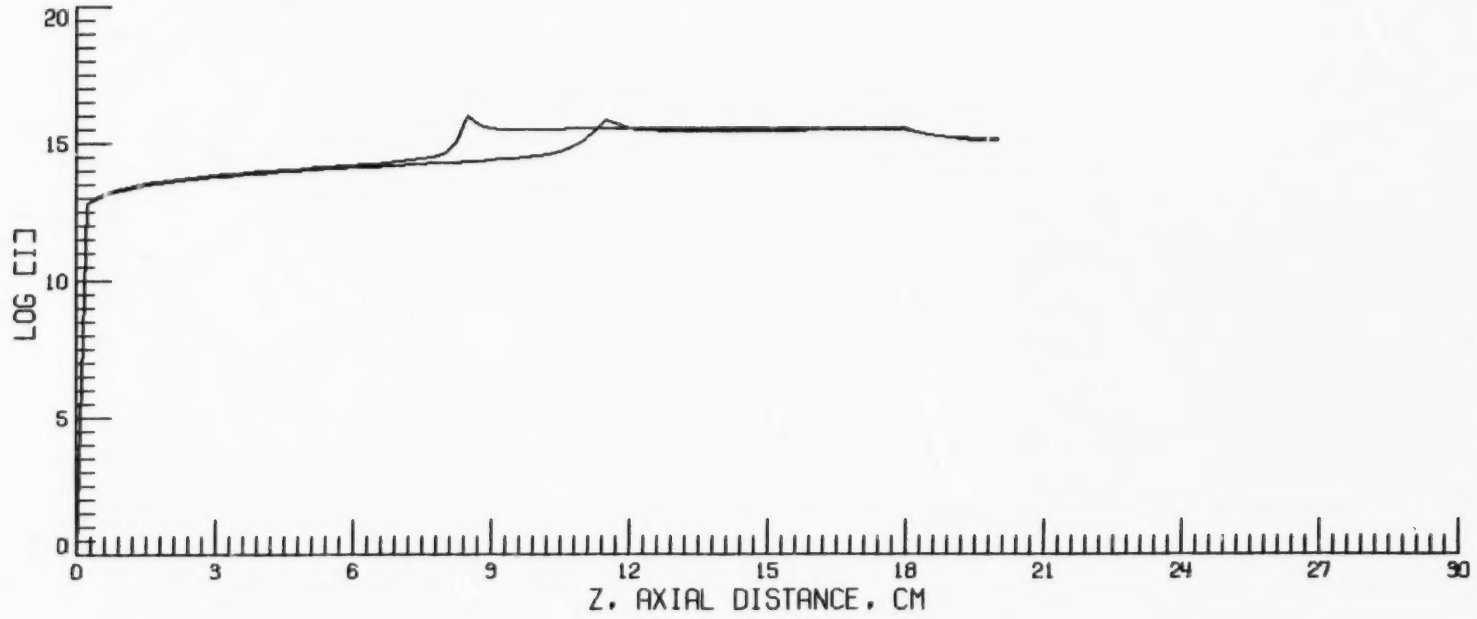
INFOPLT 1



INFOPLT 2.



INFOPLT 3.



INFOPLT 4.

INFOPLT 5.

+,-LOG(ABS(C1*J-.5*C1J))
20
10
0
-10
-20
0
3
6
9
12
15
18
21
24
27
30
Z, AXIAL DISTANCE, CM